bis-[3,3-(2-Methylpropanol-1)] disulfide

Inchi: InChI=1S/C8H18O2S2/c1-7(3-9)5-11-12-6-8(2)4-10/h7-10H,3-6H2,1-2H3
InchiKey: CIGKJLHBHYZCPS-UHFFFAOYSA-N
Formula: C8H18O2S2
SMILES: CC(CO)CSSCC(C)CO
Mol. weight [g/mol]: 210.36

Physical Properties

Property code	Value	Unit	Source
gf	-195.80	kJ/mol	Joback Method
hf	-439.73	kJ/mol	Joback Method
hfus	25.87	kJ/mol	Joback Method
hvap	79.62	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.625		Crippen Method
mcvol	168.020	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	703.48	K	Joback Method
tc	894.37	K	Joback Method
tf	340.36	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.06	J/mol×K	703.48	Joback Method
cpg	457.66	J/mol×K	735.29	Joback Method
cpg	467.66	J/mol×K	767.11	Joback Method
cpg	477.08	J/mol×K	798.92	Joback Method
cpg	485.92	J/mol×K	830.74	Joback Method
cpg	494.20	J/mol×K	862.55	Joback Method
cpg	501.92	J/mol×K	894.37	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R63138&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume